Variational data assimilation of soil moisture and temperature from remote sensing observations

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Abstract Soil moisture is a key variable for weather and climate prediction, flood forecasting, and the determination of groundwater recharge. But uncertainties related to the heterogeneity of the land surface and the non-linearity of land-atmosphere interactions severely limit our ability to accurately model and predict soil moisture on regional or continental scales. Remote-sensing techniques, on the other hand, can only indirectly measure surface soil moisture, and the data are of limited resolution in space and time. We present a "weak constraint" variational data assimilition algorithm which takes into account model as well as measurement uncertainties and optimally combines the information from both the model and the data by minimizing a least-squares performance index. We achieve a dynamically consistent interpolation and extrapolation of the remote sensing data in space and in time, or, equivalently, a continuous update of the model predictions from the data. The algorithm is tested with a synthetic experiment which is designed to mimick the conditions during the 1997 Southern Great Plains (SGP97) experiment in central Oklahoma, USA. A synthetic experiment is best suited to evaluate the performance of the algorithm as the uncertain inputs are known by design. Our data assimilation algorithm is capable of capturing quite well the spatial patterns that arise from the heterogeneity in soil types and the meteorological forcing.

INTRODUCTION

Soil moisture storage at the surface and at depth is a key variable for weather and climate prediction, flood forecasting, and the determination of groundwater recharge. Exfiltration and infiltration fronts are partially controlled by the state of the soil. In addition, the diurnal amplitudes of surface flux and state variations are affected by the conditions below the surface. There are, however, severe limitations on monitoring conditions below the surface. In-situ point measurements are inadequate for characterizing large-scale fields, and remotely-sensed passive microwaves can only be related to soil moisture in a 5 cm surface layer.

Dynamically consistent estimates of profile soil moisture may be derived through the assimilation of remotely-sensed passive microwaves into a model for moisture and temperature dynamics. Basically, the objective is to estimate soil moisture and temperature at specified times and locations. These estimates are derived from noisy scattered observations of L-band (1.4GHz) brightness temperature. Given certain assumptions, the estimation process can be reduced to the solution of a constrained least-squares problem. This problem is difficult because the number of unknowns can be very large and the constraining model is highly nonlinear.

Many of the existing soil moisture data assimilation studies focus on one-dimensional problems, eg. (Entekhabi *et al.*, 1994; Galantowicz *et al.*, 1999). Since in one dimension the number of nodes is usually very small, these studies apply *optimal* assimilation techniques such as the Kalman filter. A second category of soil moisture data assimilation studies confronts the problem of estimating horizontal as well as vertical variations in soil moisture. In order to deal with computational limitations these studies use simplified and therefore *suboptimal* estimation algorithms. Most recently, Houser *et al.* (1998) have investigated various suboptimal sequential algorithms.

DATA ASSIMILATION ALGORITHM

Our approach to the data assimilation problem is summarized in McLaughlin (1995) and Reichle *et al.* (1999). For the highly non-linear soil moisture problem, variational methods are particularly well-suited. A variational algorithm estimates the initial states and model errors for the time period between several brightness observations. The approach has been widely used in oceanographic research and in operational weather forecasting (Bennett, 1992; Thépaut & Courtier, 1991).

It is important to realize that neither the model nor the micrometeorological inputs are perfect descriptions of reality. Therefore, we account for model errors by treating the forcings as random fields which are correlated over time and space. In other words, we impose the model as a “weak constraint” only.

Assembling the soil moisture and temperature at all grid points into the state vector Y, the hydrologic model can be expressed as

$$\frac{\partial Y}{\partial t} = \varphi(Y) + \omega \qquad\qquad Y|_{t=0} = Y_0(\beta) \tag{1}$$

The right-hand side operator φ is non-linear and contains all deterministic forcings such as the observed micrometeorological inputs. The unknown stochastic model error is denoted with ω. The initial condition is parameterized with the uncertain vector β. We specify mean values $\overline{\omega}$ and $\overline{\beta}$ as well as covariances C_ω and C_β which reflect the information we have prior to using the remote sensing data. The uncertain inputs are then adjusted to minimize a weighted least-squares (Bayesian) performance measure J which attempts to provide a good fit to the measurements while respecting prior information.

$$\begin{aligned} J = {} & (Z - M[Y])^T \, C_v^{-1} \, (Z - M[Y]) \\ & + \left(\beta - \overline{\beta}\right)^T C_\beta^{-1} \left(\beta - \overline{\beta}\right) + \int_0^{t_f}\int_0^{t_f} \omega(t')^T C_\omega^{-1}(t',t'')\omega(t'')dt'dt'' \\ & + 2\int_0^{t_f} \lambda^T \left(\frac{\partial Y}{\partial t} - \varphi(Y) - \omega\right) dt + 2\lambda_0^T \left(Y|_{t=0} - Y_0(\beta)\right) \end{aligned} \tag{2}$$

The first term takes into account the misfit between the data vector Z and the measurement predictions $M[Y]$, weighted with the covariance of the measurement error covariance C_v. The second and third terms penalize deviations of the uncertain inputs from the prior means (we assume $\overline{\omega} \equiv 0$). By adjoining the state equation to the performance index with Lagrange multipliers λ (last two terms) we ensure that the estimates are dynamically consistent.

The optimal estimates of the uncertain inputs and states are obtained by setting the first variation of the adjoined performance measure equal to zero. This yields a set of socalled Euler-Lagrange equations which constitute a two-point boundary value problem.

$$\frac{\partial \hat{Y}}{\partial t} = \varphi(\hat{Y}) + \hat{\omega} \qquad \hat{Y}|_{t=0} = Y_0(\hat{\beta}) \tag{3}$$

$$-\frac{\partial \lambda}{\partial t} = \widehat{\frac{\partial \varphi}{\partial Y}}^T \lambda + \text{impulses} \qquad \lambda|_{t=t_f} = 0 \tag{4}$$

$$\hat{\omega} = \int_0^{t_f} C_\omega(t,t')\lambda(t')dt' \qquad \hat{\beta} = \overline{\beta} + C_\beta \widehat{\frac{\partial Y_0}{\partial \beta}}^T \lambda|_{t=0} \tag{5}$$

Estimates are denoted with a hat. Equation (3) expresses the fact that the estimates obey the state equation (1) and are therefore dynamically consistent. The impulses in equation (4) for the Lagrange multipliers are proportional to the misfit between the data Z and the measurement predictions $M[\hat{Y}]$. Finally, the update equation (5) relates the Lagrange multipliers to the estimates of the uncertain inputs. We solve the Euler-Lagrange equations with an iterated representer algorithm (Bennett, 1992).

Although the computational effort required is considerable, it is possible to assimilate large data sets with this method. Through its implicit propagation of the error covariances, the algorithm is very efficient and thus able to provide *optimal* estimates without the simplifications that have been used in other large-scale soil moisture estimation applications. The result is a physically consistent four-dimensional picture of the soil moisture and soil temperature fields. Additional assimilation products can include estimates of fluxes of interest to atmospheric scientists, hydrologists, and ecologists.

SOIL MOISTURE MODELLING

The feasibility of large-scale soil moisture data assimilation is highly dependent on our ability to develop computationally efficient models which capture the key physical processes that relate near-surface soil moisture to remotely-sensed brightness measurements. Consequently, we have specifically designed our model for data assimilation purposes.

Our model of coupled moisture and heat transport is based on ideas described by Ács *et al.* (1991). Soil moisture transport is described with Richards' equation. We use the formulation by Clapp & Hornberger (1978) for the soil hydraulic properties. Currently we use six subsurface layers in the vertical (0–5 cm, 5–15 cm, 15–30 cm, 30–45 cm, 45–60 cm, and 60–90 cm). In order to achieve maximum computational efficiency, we use the force-restore method (Hu & Islam, 1995) rather than the full heat equation to describe temperature dynamics. As the brightness temperature depends only on the soil temperature in the top layer, the force-restore approximation is ideally suited for our goal to infer soil moisture from brightness observations. At the land surface, we assume neutral conditions and compute atmospheric fluxes with a resistance formulation. The vegetation submodel is designed after the Simplified Biosphere Model (SSiB) (Xue *et al.*, 1991). The downward flux out of the bottom soil layer is described by gravitational drainage. The brightness temperature is related to the system states with a Radiative Transfer model similar to the one described by Galantowicz *et al.* (1999).

Since for agricultural regions with modest relief the vertical fluxes dominate in the unsaturated zone, our approach is to neglect unsaturated horizontal moisture and heat transport. The vertical soil columns for different pixels have different soil properties and meteorological inputs. But such inputs do not vary arbitrarily from pixel to pixel. Instead, they typically exhibit spatial structure (or correlation) which reflects the effect of larger-scale geological or meteorological processes. We account for this structure by using an exponential correlation for the error covariances C_ω and C_β. For the time correlation of C_ω we also use an exponential function.

Our model has been tested by comparing its predictions with measurements from the BARC data set (Jackson *et al.*, 1997). These tests show that the model with the above-mentioned discretization is able to simulate soil moisture and temperature variations over time and space with appropriate accuracy. We believe that the model described here is sufficiently accurate and computationally efficient to form the basis for an operational soil moisture data assimilation algorithm.

SYNTHETIC EXPERIMENT

The synthetic test problem is based on the recent Southern Great Plains (SGP97) field experiment. The area chosen for the synthetic experiment is shown in Fig. 1. It ranges from $-98.4°$ to $-97.5°$ West and from $34.5°$ to $36°$ North, which is a rectangular area of 80 km $\times$ 160 km (UTM Zone 14 projection). We divide this area into 16 by 32 pixels of 5 km $\times$ 5 km, ie. a total number of 512 pixels. On each of these pixels, the soil moisture and temperature profiles are estimated. The soil data have been compiled from the ESSC data base at Pennsylvania State University [*http://www.essc.psu.edu*]. The meteorological inputs are taken from the Oklahoma Mesonet database [*http://okmesonet.ocs.ou.edu*]. The experiment covers a four-week period from June 18, 1997 (day of year 169) to July 15, 1997 (day of year 196).

For the synthetic experiment, we generate a time series of model error fields ω and initial condition parameters β to obtain a "true" solution from (1). The corresponding "prior" solution is the solution of (1) with the model error and the initial condition parameters set to their prior values $\overline{\omega} \equiv 0$ and $\overline{\beta}$, respectively. The prior solution is our best guess prior to using the remotely-sensed brightness data. We also generate a sequence of observation error fields (5 K standard deviation) to obtain the synthetic remote sensing data Z. From the noisy data Z (one brightness image per day) and the prior solution, the data assimilation algorithm estimates soil moisture and temperature profiles. We then compare the estimate and the prior to the true solution.

Fig. 2 compares a sequence of spatial plots of the true and the estimated top node soil moisture. Our intentionally poor prior guess of the initial top node saturation is 0.5 everywhere in the domain. Obviously, the algorithm is capable of capturing quite well the spatial patterns that arise from the initial condition as well as from the heterogeneity in soil types and meteorological forcing.

Finally, Fig. 3 shows some typical vertical profiles. Clearly, the effect of the assimilation of the brightness data is to improve our knowledge of the true soil moisture. It is also obvious how the model interpolates between the observation times and extrapolates into the deeper soil in a physically consistent way. This is a huge advantage over soil moisture fields that are derived by direct inversion of brightness fields without the use of a dynamic data assimilation scheme.

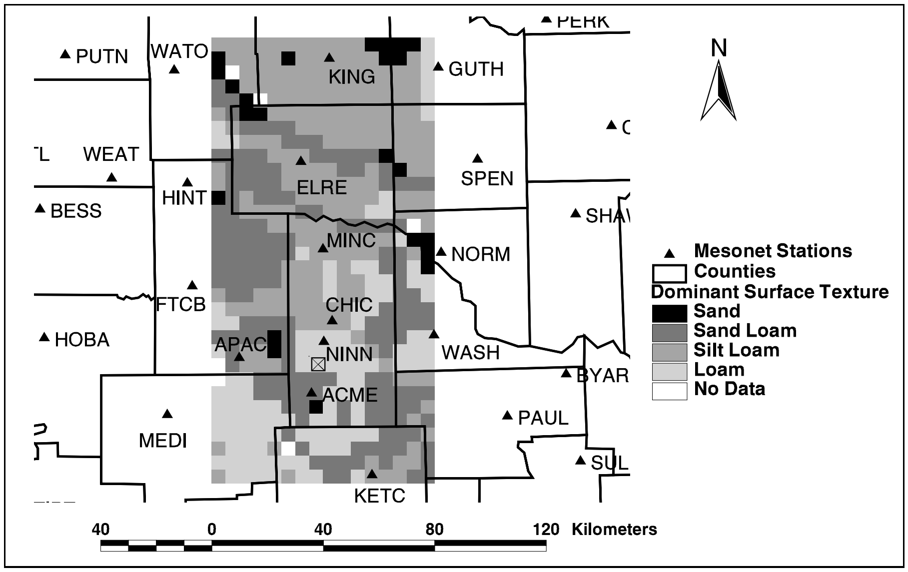

Fig. 1 Experiment area for the synthetic test problem. Also shown are the dominant surface texture class for each pixel and the Mesonet stations. Note the marked estimation pixel (south-west of Mesonet station NINN), for which profiles of soil moisture are shown in Fig. 3.

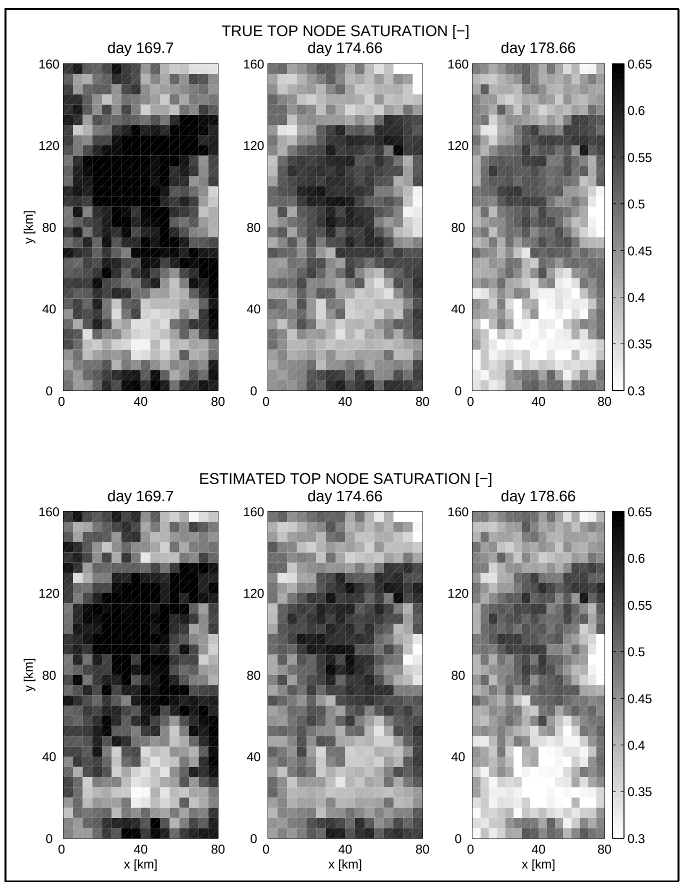

Fig. 2 True (top row) and estimated (bottom row) top node saturation for three different times during the 28-day estimation window.

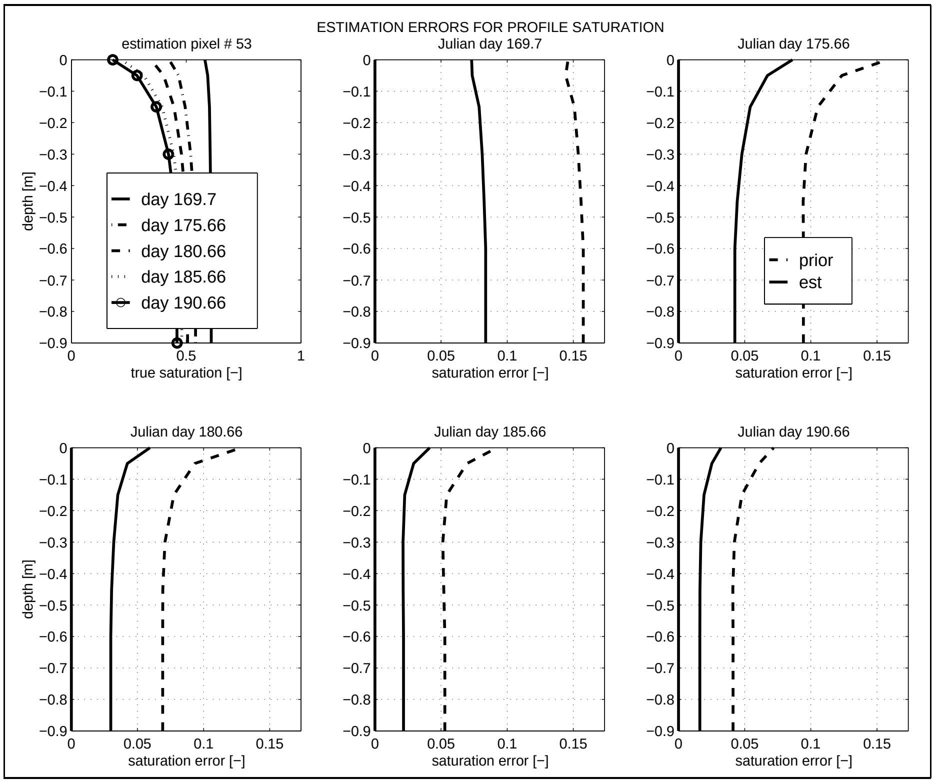

Fig. 3 Saturation profiles and errors for the pixel marked in Fig. 1. In the first graph, the true profiles are plotted for five particular times (mornings) during the 28-day estimation window. In the other five graphs, the prior and the estimation errors in the saturation profile are shown for the same five times.

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